**Program:** Chemistry (15025012071P6)

**Course:** COMPUTATIONAL CHEMISTRY

**Code:** PPGQU0049

**Workload:** 60 hours

**Credits:** 04

**Syllabus:**

Review of Quantum Mechanics; The Hartree-Fock Method; Molecular Orbital Theory; Construction of Basis Sets; Post-Hartree-Fock Correlated Methods; Density Functional Theory; Current Methods.

**Bibliography:**

Jensen, F. Introduction to Computational Chemistry, John Wiley & Sons, New York, 2002.

Cramer, C.J. Essentials of Computational Chemistry: Theories and Models, 2nd ed., John Wiley & Sons, New York, 2002.

Szabo, A.; Ostlund, N. S. Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Dover Publications, New York, 1989.

Foresman, J.B.; Frisch, A. Exploring Chemistry with Electronic Structure Methods: A Guide to Using Gaussian, Gaussian Inc., 1993.

Recent articles from the literature.